Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:42 PM GMT

PDB ID : 3RQE
Title : Cerebral cavernous malformation 3 (CCM3) in complex with paxillin LD1
Authors : Li, X.; Zhang, R.; Boggon, T.J.
Deposited on : 2011-04-28
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:
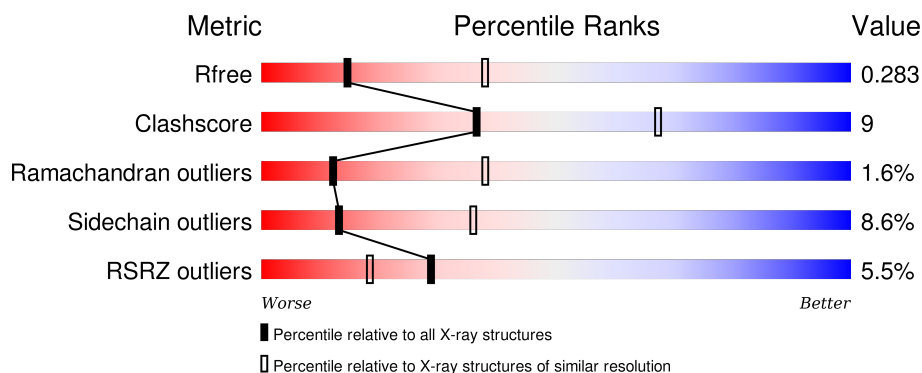
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	214	6% 62% 22% 5% 11%
1	B	214	6% 68% 21% • 10%
1	C	214	5% 71% 20% • 5%
1	D	214	3% 59% 24% • 13%
2	E	14	14% 57% 14% 29%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6351 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Programmed cell death protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total 1550	C 990	N 263	O 292	S 5	0	0	0
1	B	192	Total 1567	C 1002	N 264	O 295	S 6	0	0	0
1	C	203	Total 1644	C 1042	N 278	O 314	S 10	0	0	0
1	D	187	Total 1518	C 972	N 253	O 288	S 5	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q9BUL8
A	0	HIS	-	EXPRESSION TAG	UNP Q9BUL8
B	-1	GLY	-	EXPRESSION TAG	UNP Q9BUL8
B	0	HIS	-	EXPRESSION TAG	UNP Q9BUL8
C	-1	GLY	-	EXPRESSION TAG	UNP Q9BUL8
C	0	HIS	-	EXPRESSION TAG	UNP Q9BUL8
D	-1	GLY	-	EXPRESSION TAG	UNP Q9BUL8
D	0	HIS	-	EXPRESSION TAG	UNP Q9BUL8

- Molecule 2 is a protein called Paxillin LD1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	10	Total 72	C 44	N 10	O 18	0	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Programmed cell death protein 10
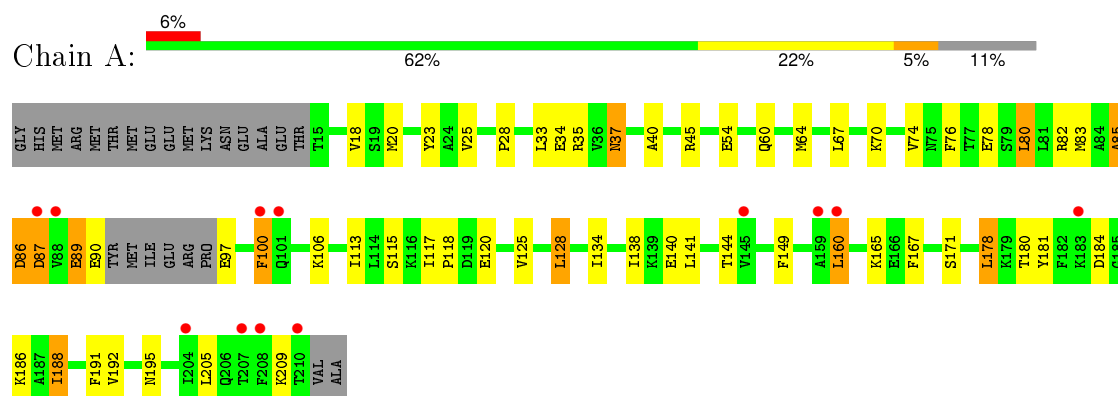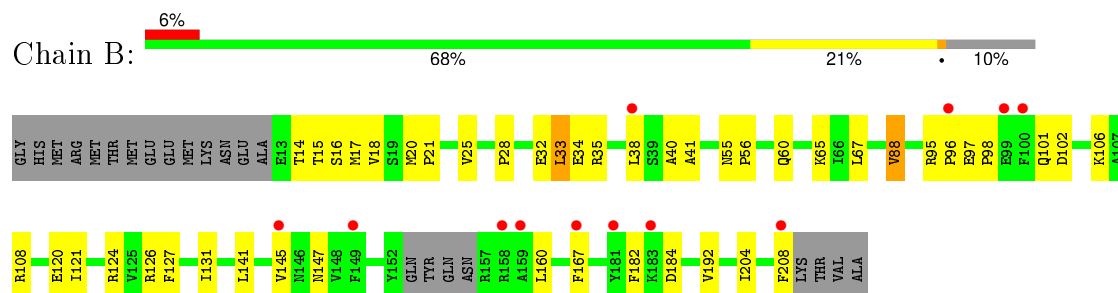
- Molecule 1: Programmed cell death protein 10

- Molecule 1: Programmed cell death protein 10

- Molecule 1: Programmed cell death protein 10

GLY HIS MET ARG MET THR MET GLU GLU MET LYS ASN GLU A12 E13 T14 V18 P21 L33 N37 L38 Q42 T43 L44 A51 N55 L58 T59 Q60 I63 M64 K70 V74 E78 R82 V88 Y91 MET ILE GLU ARG PRO E97 P98 E99

F100 N104 A107 R108 Q112 K116 E120 D123 R124 V125 R126 Q129 T130 D133 I134 I138 L141 L142 D143 F149 K150 K151 Y152 GLN TYR GLN ASN ARG R158 A159 L160 Q163 K164 K165 E166 F167 V168 K169 Y170 S173 F174 S175 D176 T177 F182

A187 I188 N189 V190 S193 L197 Q200 T201 N202 L203 T207 F208 LYS THR VAL ALA
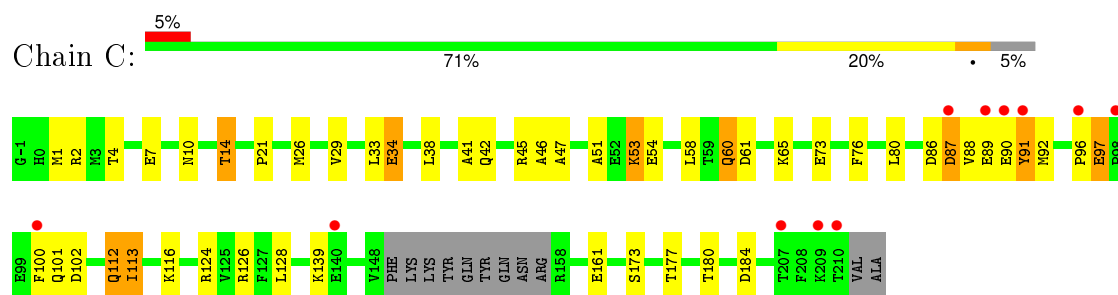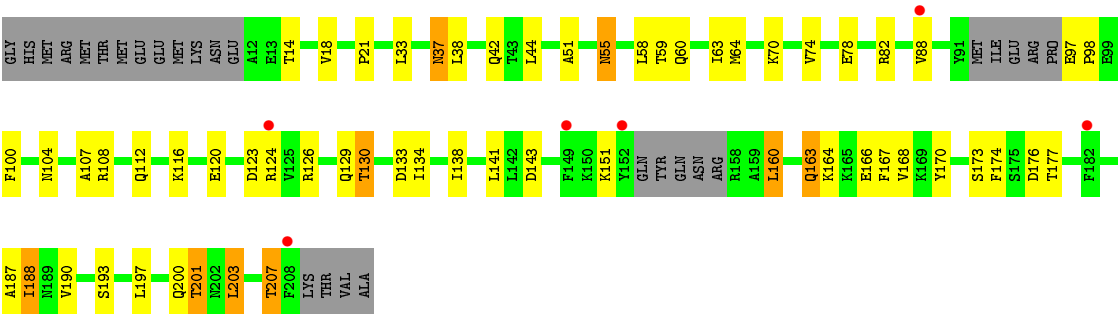
• Molecule 2: Paxillin LD1 peptide

Chain E:

14%

57% 14% 29%

ASP ASP LEU D5 A6 L7 L8 L11 T14 THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.16Å 117.99Å 123.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.92 – 2.80 38.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.92-2.80) 99.9 (38.92-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.240 , 0.295 0.234 , 0.283	Depositor DCC
R_{free} test set	1192 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	71.4	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.5	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 23402 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6351	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.56	0/1572	0.66	0/2113
1	B	0.53	0/1590	0.62	0/2138
1	C	0.56	0/1666	0.64	0/2238
1	D	0.55	0/1539	0.65	0/2069
2	E	0.38	0/71	0.74	0/96
All	All	0.55	0/6438	0.64	0/8654

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1550	0	1592	31	0
1	B	1567	0	1609	27	0
1	C	1644	0	1683	36	0
1	D	1518	0	1554	37	0
2	E	72	0	68	1	0
All	All	6351	0	6506	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ARG:H	1:C:42:GLN:HE22	1.20	0.89
1:C:2:ARG:H	1:C:42:GLN:NE2	1.72	0.86
1:A:141:LEU:O	1:A:144:THR:HG22	1.86	0.76
1:B:32:GLU:HA	1:B:35:ARG:HH11	1.55	0.71
1:C:89:GLU:O	1:C:92:MET:HG2	1.91	0.70
1:D:197:LEU:O	1:D:201:THR:HG23	1.93	0.69
1:A:74:VAL:HG22	1:A:188:ILE:HG23	1.77	0.66
1:D:97:GLU:HB2	1:D:100:PHE:HD2	1.60	0.66
1:C:97:GLU:HG3	1:C:100:PHE:HB2	1.78	0.65
1:C:10:ASN:O	1:C:14:THR:CG2	2.45	0.65
1:B:33:LEU:HG	1:B:41:ALA:HB2	1.77	0.65
1:B:33:LEU:HD12	1:B:33:LEU:O	2.00	0.61
1:A:89:GLU:O	1:A:90:GLU:HB2	2.00	0.61
1:D:170:TYR:CD2	1:D:200:GLN:NE2	2.70	0.59
1:B:55:ASN:O	1:B:56:PRO:C	2.40	0.59
1:D:37:ASN:C	1:D:37:ASN:HD22	2.05	0.59
1:A:37:ASN:ND2	1:A:40:ALA:H	2.00	0.59
1:A:188:ILE:O	1:A:192:VAL:HG23	2.03	0.58
1:D:97:GLU:HB2	1:D:100:PHE:CD2	2.40	0.56
1:A:33:LEU:O	1:A:35:ARG:N	2.39	0.55
1:D:51:ALA:HB1	1:D:58:LEU:HD23	1.89	0.54
1:C:1:MET:HE1	1:C:45:ARG:HB2	1.88	0.54
1:A:85:ALA:HB2	1:A:115:SER:CB	2.38	0.54
1:C:51:ALA:HB1	1:C:58:LEU:HD23	1.90	0.54
1:C:10:ASN:O	1:C:14:THR:HG23	2.06	0.54
1:B:121:ILE:HG13	1:B:121:ILE:O	2.08	0.54
1:C:10:ASN:O	1:C:14:THR:HG22	2.07	0.53
1:A:85:ALA:O	1:A:86:ASP:C	2.45	0.53
1:C:97:GLU:CG	1:C:100:PHE:HB2	2.38	0.53
1:C:47:ALA:HB1	1:D:44:LEU:HD23	1.91	0.52
1:A:134:ILE:O	1:A:138:ILE:HG13	2.09	0.52
1:C:4:THR:OG1	1:C:7:GLU:HG3	2.10	0.52
1:D:129:GLN:NE2	1:D:133:ASP:OD2	2.43	0.52
1:B:21:PRO:HG2	1:B:60:GLN:HB2	1.92	0.52
1:C:180:THR:O	1:C:184:ASP:HB2	2.10	0.52
1:C:51:ALA:HB1	1:C:58:LEU:CD2	2.40	0.52
1:B:88:VAL:HG13	1:B:108:ARG:CG	2.41	0.51
1:D:167:PHE:CD2	1:D:167:PHE:C	2.83	0.51
1:D:126:ARG:O	1:D:130:THR:OG1	2.29	0.51
1:C:33:LEU:HD11	1:D:58:LEU:HD11	1.92	0.51
1:A:205:LEU:O	1:A:209:LYS:HB2	2.11	0.50
1:D:59:THR:O	1:D:63:ILE:HG12	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ARG:O	1:C:128:LEU:HB2	2.12	0.50
1:A:125:VAL:O	1:A:128:LEU:HB3	2.11	0.50
1:D:74:VAL:HG13	1:D:188:ILE:HG23	1.93	0.50
1:B:16:SER:HB3	1:B:18:VAL:HG22	1.93	0.50
1:A:149:PHE:HE1	1:A:160:LEU:HB3	1.77	0.50
1:D:173:SER:O	1:D:176:ASP:HB2	2.12	0.50
1:D:70:LYS:O	1:D:74:VAL:HG23	2.12	0.49
1:B:141:LEU:O	1:B:145:VAL:HG23	2.12	0.49
1:D:203:LEU:O	1:D:207:THR:OG1	2.24	0.49
1:A:76:PHE:CE1	1:B:20:MET:HB3	2.48	0.49
1:A:23:TYR:O	1:A:28:PRO:HD3	2.13	0.49
1:C:97:GLU:HG3	1:C:100:PHE:CD2	2.49	0.48
1:A:106:LYS:HE3	1:A:140:GLU:HB3	1.95	0.48
1:C:1:MET:HE1	1:C:45:ARG:CB	2.44	0.48
1:C:88:VAL:O	1:C:92:MET:HB3	2.14	0.48
1:D:38:LEU:HG	1:D:42:GLN:NE2	2.28	0.48
1:D:174:PHE:HA	1:D:193:SER:OG	2.13	0.47
1:A:141:LEU:HD23	1:A:167:PHE:CZ	2.49	0.47
1:C:1:MET:HG3	1:C:34:GLU:HG3	1.95	0.47
1:B:98:PRO:HA	1:B:101:GLN:HB2	1.96	0.47
1:A:67:LEU:HD23	1:B:67:LEU:HD23	1.97	0.47
1:C:76:PHE:CZ	1:C:80:LEU:HD21	2.49	0.47
1:A:188:ILE:HA	1:A:191:PHE:CD2	2.50	0.47
1:D:120:GLU:HA	1:D:120:GLU:OE2	2.14	0.46
1:D:78:GLU:O	1:D:82:ARG:HG3	2.15	0.46
1:B:32:GLU:HA	1:B:35:ARG:NH1	2.27	0.46
1:A:178:LEU:O	1:A:181:TYR:HB3	2.15	0.46
1:A:184:ASP:HB3	1:A:186:LYS:H	1.81	0.46
1:B:124:ARG:HG2	1:B:182:PHE:HE1	1.80	0.46
1:A:60:GLN:HA	1:A:60:GLN:HE21	1.81	0.46
1:C:113:ILE:H	1:C:113:ILE:HG12	1.58	0.46
1:D:160:LEU:HD12	1:D:207:THR:HG22	1.98	0.46
1:A:78:GLU:O	1:A:82:ARG:HG3	2.17	0.45
1:D:107:ALA:HA	1:D:141:LEU:HD13	1.98	0.45
1:B:95:ARG:HA	1:B:96:PRO:HD3	1.84	0.45
1:A:25:VAL:O	1:A:28:PRO:HD2	2.16	0.45
1:D:177:THR:HG21	1:D:190:VAL:HA	1.99	0.45
1:A:83:MET:CE	1:B:17:MET:SD	3.05	0.44
1:C:112:GLN:O	1:C:116:LYS:HG3	2.18	0.44
1:D:21:PRO:HG2	1:D:60:GLN:HE21	1.81	0.44
1:D:134:ILE:O	1:D:138:ILE:HG13	2.17	0.44

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE3	1:C:41:ALA:C	2.38	0.44
1:D:164:LYS:O	1:D:168:VAL:HG23	2.18	0.44
1:C:53:LYS:HG3	1:C:54:GLU:N	2.29	0.43
1:B:33:LEU:HD11	1:B:40:ALA:HB3	2.01	0.43
1:B:88:VAL:HG13	1:B:108:ARG:HG2	1.99	0.43
1:D:197:LEU:O	1:D:201:THR:CG2	2.64	0.43
1:B:88:VAL:HG13	1:B:108:ARG:HG3	2.00	0.43
1:D:55:ASN:O	1:D:58:LEU:HB2	2.19	0.43
1:C:26:MET:O	1:C:29:VAL:HB	2.17	0.43
1:C:96:PRO:HA	1:C:101:GLN:CG	2.48	0.42
1:B:167:PHE:HB2	1:B:204:ILE:HD11	1.99	0.42
1:C:58:LEU:HD11	1:D:33:LEU:HD21	2.01	0.42
1:D:187:ALA:O	1:D:190:VAL:N	2.50	0.42
1:C:21:PRO:HG2	1:C:60:GLN:HB2	2.00	0.42
1:B:127:PHE:O	1:B:131:ILE:HG12	2.20	0.42
1:C:139:LYS:HA	2:E:8:LEU:HD21	2.00	0.42
1:A:64:MET:CE	1:B:192:VAL:HG21	2.50	0.42
1:A:67:LEU:HD23	1:B:67:LEU:CD2	2.50	0.41
1:C:73:GLU:CD	1:D:60:GLN:HE22	2.24	0.41
1:B:34:GLU:HG2	1:B:38:LEU:HD23	2.02	0.41
1:D:177:THR:HG22	1:D:190:VAL:HG22	2.02	0.41
1:A:76:PHE:CE2	1:A:80:LEU:HD22	2.55	0.41
1:C:61:ASP:O	1:C:65:LYS:HG3	2.20	0.41
1:D:51:ALA:HB1	1:D:58:LEU:CD2	2.51	0.41
1:A:85:ALA:HB2	1:A:115:SER:HB3	2.02	0.41
1:C:7:GLU:OE2	1:C:46:ALA:CB	2.69	0.41
1:B:25:VAL:C	1:B:28:PRO:HD2	2.40	0.41
1:C:1:MET:HE3	1:C:42:GLN:HA	2.02	0.41
1:A:60:GLN:HA	1:A:60:GLN:NE2	2.36	0.41
1:D:163:GLN:O	1:D:166:GLU:N	2.53	0.41
1:C:86:ASP:HB3	1:C:87:ASP:H	1.61	0.41
1:D:38:LEU:O	1:D:42:GLN:HG3	2.21	0.40
1:D:60:GLN:O	1:D:64:MET:HG2	2.20	0.40
1:D:123:ASP:HB3	1:D:126:ARG:HB2	2.03	0.40
1:A:97:GLU:HB2	1:A:100:PHE:HD2	1.87	0.40
1:C:91:TYR:CD1	1:C:91:TYR:N	2.89	0.40
1:A:117:ILE:N	1:A:118:PRO:CD	2.83	0.40
1:B:121:ILE:HD12	1:B:127:PHE:CZ	2.57	0.40
1:B:102:ASP:O	1:B:106:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	186/214 (87%)	164 (88%)	17 (9%)	5 (3%)	6	21
1	B	188/214 (88%)	167 (89%)	20 (11%)	1 (0%)	34	69
1	C	199/214 (93%)	184 (92%)	13 (6%)	2 (1%)	19	52
1	D	181/214 (85%)	160 (88%)	17 (9%)	4 (2%)	8	28
2	E	8/14 (57%)	8 (100%)	0	0	100	100
All	All	762/870 (88%)	683 (90%)	67 (9%)	12 (2%)	12	38

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	85	ALA
1	C	34	GLU
1	C	87	ASP
1	A	70	LYS
1	A	87	ASP
1	D	151	LYS
1	A	86	ASP
1	B	147	ASN
1	D	207	THR
1	D	124	ARG
1	D	98	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	173/194 (89%)	154 (89%)	19 (11%)	8	23
1	B	175/194 (90%)	164 (94%)	11 (6%)	22	53
1	C	184/194 (95%)	170 (92%)	14 (8%)	16	42
1	D	169/194 (87%)	153 (90%)	16 (10%)	11	30
2	E	8/12 (67%)	7 (88%)	1 (12%)	6	17
All	All	709/788 (90%)	648 (91%)	61 (9%)	13	36

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	VAL
1	A	20	MET
1	A	37	ASN
1	A	45	ARG
1	A	54	GLU
1	A	80	LEU
1	A	87	ASP
1	A	89	GLU
1	A	100	PHE
1	A	113	ILE
1	A	120	GLU
1	A	128	LEU
1	A	160	LEU
1	A	165	LYS
1	A	171	SER
1	A	178	LEU
1	A	180	THR
1	A	188	ILE
1	A	195	ASN
1	B	14	THR
1	B	15	THR
1	B	33	LEU
1	B	65	LYS
1	B	88	VAL
1	B	97	GLU
1	B	120	GLU
1	B	126	ARG
1	B	160	LEU
1	B	184	ASP
1	B	208	PHE
1	C	14	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	38	LEU
1	C	53	LYS
1	C	60	GLN
1	C	90	GLU
1	C	91	TYR
1	C	97	GLU
1	C	102	ASP
1	C	112	GLN
1	C	113	ILE
1	C	126	ARG
1	C	161	GLU
1	C	173	SER
1	C	177	THR
1	D	14	THR
1	D	18	VAL
1	D	37	ASN
1	D	55	ASN
1	D	88	VAL
1	D	104	ASN
1	D	108	ARG
1	D	112	GLN
1	D	116	LYS
1	D	130	THR
1	D	143	ASP
1	D	160	LEU
1	D	163	GLN
1	D	188	ILE
1	D	201	THR
1	D	203	LEU
2	E	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	60	GLN
1	A	104	ASN
1	A	189	ASN
1	B	55	ASN
1	B	60	GLN
1	B	75	ASN
1	B	101	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	42	GLN
1	C	55	ASN
1	C	60	GLN
1	C	112	GLN
1	D	37	ASN
1	D	42	GLN
1	D	60	GLN
1	D	112	GLN
1	D	189	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	190/214 (88%)	0.31	12 (6%)	23	14	44, 81, 116, 158	0
1	B	192/214 (89%)	0.31	12 (6%)	23	14	39, 84, 157, 186	0
1	C	203/214 (94%)	0.17	11 (5%)	29	19	38, 74, 150, 178	0
1	D	187/214 (87%)	0.14	6 (3%)	51	39	39, 78, 148, 180	0
2	E	10/14 (71%)	1.19	2 (20%)	1	1	164, 186, 228, 234	0
All	All	782/870 (89%)	0.25	43 (5%)	29	18	38, 80, 152, 234	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	210	THR	6.8
1	C	100	PHE	6.3
1	B	100	PHE	5.4
1	C	89	GLU	4.5
1	C	96	PRO	4.3
1	A	210	THR	4.1
1	A	208	PHE	4.0
2	E	6	ALA	3.8
1	A	100	PHE	3.7
1	C	98	PRO	3.7
1	B	159	ALA	3.7
1	B	145	VAL	3.4
1	A	145	VAL	3.3
1	B	183	LYS	3.3
1	C	87	ASP	3.2
1	D	152	TYR	3.2
1	D	124	ARG	3.1
1	D	149	PHE	3.0
2	E	5	ASP	3.0
1	A	159	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	88	VAL	2.9
1	B	149	PHE	2.8
1	A	87	ASP	2.8
1	D	208	PHE	2.8
1	A	160	LEU	2.7
1	A	207	THR	2.7
1	A	183	LYS	2.6
1	B	167	PHE	2.6
1	C	207	THR	2.6
1	C	209	LYS	2.5
1	D	88	VAL	2.5
1	C	91	TYR	2.4
1	A	101	GLN	2.4
1	B	181	TYR	2.4
1	C	90	GLU	2.3
1	C	140	GLU	2.3
1	B	158	ARG	2.2
1	A	204	ILE	2.2
1	B	38	LEU	2.1
1	D	182	PHE	2.1
1	B	208	PHE	2.1
1	B	96	PRO	2.0
1	B	99	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.